

## INSIDE

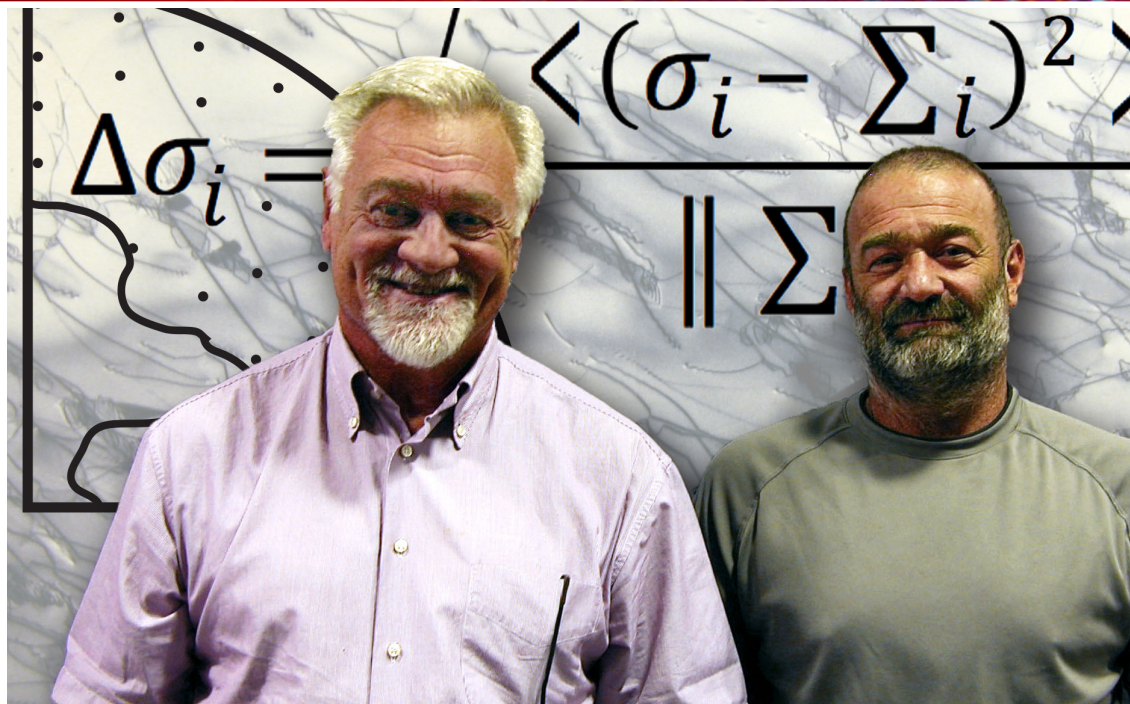
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Carlos Tomé (left) and Ricardo Lebensohn recently saw their viscoplastic self-consistent code (in background) research reach 1,000 citations in Google Scholar.

## Carlos Tomé and Ricardo Lebensohn

*Developers of a long-standing,  
versatile code and collaboration*

*By Diana Del Mauro, ADEPS Communications*

When they first met in 1985 at Argentina's Universidad Nacional de Rosario, Ricardo Lebensohn was an enthusiastic undergraduate physics student and Carlos Tomé an earnest first-year professor. After taking Tomé's statistical mechanics course, Lebensohn asked him to be his graduate school advisor. Through his PhD dissertation project—the development of a computational code to reliably simulate materials behavior—he forged a bond with Tomé that has stood the test of time and produced valuable, award-winning work.

"It all started with Ricardo's PhD and we expanded the code through the years," said Tomé, noting that their co-authored 1993 *Acta Metallurgica et Materialia* paper, "A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: Application to zirconium alloys," recently reached the 1,000-citation mark in Google Scholar.

Drawing upon prior work by French researchers, Lebensohn reformulated the problem, making it easier and faster to

*continued on page 3*

*At Los Alamos the  
ever-evolving code enables  
science and engineer-  
ing required to establish  
novel design principles and  
manufacturing processes  
for advanced materials.*



## From Dianne's desk . . .

A few weeks ago, Karen Kippen asked me if I would be willing to write the column for this *MST e-NEWS*. She sent along a few past editions, like Anna Zurek's last column as she retired. After reading those, I got a little nervous, but here goes!

My name is Dianne Williams Wilburn. I am the new executive advisor in MST Division. I introduce myself as "the new Jim Coy," as most people in the division knew or worked with Jim. I have been at the Lab 18 years. Like a lot of people, my husband and I came here for "a few years," and like a lot of people, we are still here.

When I saw the job posting for the executive advisor position and the required job skills, I thought I had the experience and that it would be a job that I enjoyed. Based on my eight weeks in the position, I see the job as helping MST with implementing conduct of operations and any and everything related to environment, safety, and health. Some of the issues related to this topics can be fixed with a phone call, such as getting our parking lot re-striped—to things that might take a year, like getting a special type of waste documented and disposed of—to things that may take a few years if they require, say, a change in institutional policy.

Hopefully, I can help the people in MST get their jobs done by helping with meeting the conduct of operations and environment, safety, and health requirements. To find out how I can help and learn more about the work in the division, I plan to attend each team's weekly meeting a few times a year and schedule the division leaders' MOVs (management observation and verification), so they see each team at least once a year. By attending the team meetings, I am learning about things like someone who may need help tracking down the status of an engineering service request. That type of issue is something I hope in the future people will feel free to call me about.

In my short time here, my impression is that everyone has their work documented in an integrated work document, the IWD. Sure, the writing styles may differ a bit, but the steps for the work, the hazard controls, the training—it is all there. I see two things we need to do, but I don't claim to have the solution. The first is to stay on top of changing conditions—or, another way of saying this is—changes in the hazards. In our work culture—well, at home as well for that matter—we need to have the habit of asking ourselves what has changed since the last time we performed this task. The second involves feedback for continuous improvement. To me, as a member of a team reviewing the work to be done—be it in a pre-job brief or an annual review—an ideal world resulting in a safer workplace would be to have the time to ensure the paperwork reflects our ideas for improvement.

So, I hope I can help people get their work done, the projects going. A friend of mine, who has retired from the lab, once said something that has helped me along the way, not that I always practice what I preach. He said instead of getting frustrated with a new requirement or policy, he had quit responding in frustration: it wasted energy. He took the attitude that if this was the way it was to be, he figured out how he could make it work for the work he wanted to do. That sort of sums up what I hope to do.

*MST Executive Advisor Dianne Wilburn*

“

*I see the job as helping MST with implementing conduct of operations and any and everything related to environment, safety, and health ... I hope I can help people get their work done, the projects going.*

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### *Tomé and Lebensohn cont.*

investigate the behavior of metallic aggregates than with previous simulation codes, which required days to generate one result. IBM personal computers had just become powerful enough to tackle such problems, and Lebensohn wrote the viscoplastic self-consistent (VPSC) code in Fortran programming language. Graphics software not yet being available, they traced figures by hand. With a smile, Lebensohn recalled Tomé redrawing his figures, which usually weren't tidy enough for his mentor's taste.

The men fell into an efficient way of working together, one that continues as they collaborate—often conversing in Spanish with each other—as members of the Materials Science in Radiation and Dynamics Extremes (MST-8) group. “Ricardo likes to see results quickly: write code and do calculations,” Tomé said. “I have a more contemplative attitude. I like to sleep over things and let them ferment before jumping into action.”

Tomé joined the Laboratory's Center for Materials Science in 1996; Lebensohn followed in 2003. Siegfried Hecker, the center director, had launched an initiative to develop microstructural-based modeling to improve materials performance, and the VPSC approach was a good fit. Applicable to metals, minerals, and polymers, the VPSC code can help in understanding the properties of materials and inform techniques to make them inherently more reliable for the intended application and perhaps less expensive to manufacture.

At Los Alamos the ever-evolving code enables science and engineering required to establish novel design principles

and manufacturing processes for advanced materials. It has helped solve challenges in forming uranium parts. In light-water reactors—where radioactive fuel, stress variations, and temperature fluctuations can cause structural defects that grow into fracture—the code can predict dimensional changes of fuel-cladding tubes through the lifetime of the reactor—important for fuel reliability and safety.

The VPSC code can be linked with larger finite element codes or it can be used to derive physical laws that can be expressed analytically and implemented in production codes. It simulates plastic forming and predicts flow stress, texture, and microstructure evolution associated with large strain deformation. Such predictions can help control functionality of materials in extreme environments—a chief pursuit at the Laboratory. Lebensohn said he sees the code as complementary to experiments at the Laboratory's proposed Matter-Radiation Interactions in Extremes (MaRIE) facility. “Large instruments don't give you directly the measurement you want,” he said. “You need modeling to explore the microscopic mechanisms.”

The VPSC code has been distributed free of charge to more than 300 external users. Many requests come from materials scientists interested in the deformation of magnesium and from geologists wanting to infer the geological history of the Earth's interior based on signatures present in rocks' microstructure.

“If users come up with a challenging and interesting problem, we start collaborating with them,” Lebensohn said.

## **Tomé and Lebensohn's favorite computational result**

**What:** To find out if predictions from our viscoplastic self-consistent (VPSC) method could explain experimental evidence, we picked a problem that had eluded previous polycrystal codes—the ability to simulate the rolling process and the texture evolution of a zirconium alloy used in nuclear reactors.

**Why:** Texture is extremely important because it determines how reactor tubes are going to change dimensions (irradiation creep and growth) when subjected to irradiation that, in turn, affect the performance and lifetime of the reactor.

**When:** 1992 and 10 years later

**Where:** Universidad Nacional de Rosario, Argentina, and Los Alamos National Laboratory

**How:** In a few hours we got a numerical rolling texture prediction but since our desktop computer had no graphic hardware to display it, we had to send it to a remote computing center. Two days later we got the plots and, to our relief and elation, the predictions were fully consistent with the measured textures!

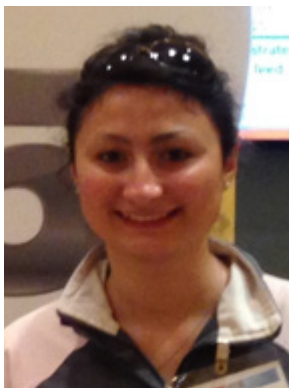
**The “a-ha moment:”** VPSC was a breakthrough for the simulation of not only zirconium but also a whole class of hexagonal metals and low symmetry materials of geologic interest. Ten years after the original zirconium simulation, and thanks to increased computational power, we were able to interface VPSC with the finite element code ABAQUS and produce simulations of complex forming operations at Los Alamos. For example, VPSC has been used to reveal physically based constitutive behavior from simulations of beam bending experiments of zirconium, titanium, and uranium, involving thousands of integration points with a representative polycrystal associated to each one, a calculation involving millions of grains and state variables.

## MST researchers in the news

### *MST-8 early-career researchers win TMS poster awards*

Eda Aydogan and M. Arul Kumar (both Materials Science and Radiation Dynamics, MST-8) won awards for their research presented in poster sessions at TMS 2015, the annual meeting and exhibition of The Minerals, Metals, & Materials Society, held recently in Florida.

Aydogan received a best poster award in the Microstructural Processes in Irradiated Materials session for “Microstructure and mechanical property evolution during tube processing of oxide dispersion strengthened (ODS) ferritic steels,” and “Swelling resistance of several variants of ferritic alloy EK-181 at high doses during self ion irradiation.”



Mentored by Osman Anderoglu and Stuart Maloy (MST-8) and pursuing a PhD in materials science from Texas A&M University, she presented new data on high-radiation tolerance of a ferritic alloy under ion irradiation and the development of tubing from radiation-tolerant, oxide-dispersion-strengthened ferritic alloys.

The Advanced Fuels Campaign of the Department of Energy's Office of Nuclear Energy's Fuel Cycle Research and Development Program funded the work, which supports the Lab's Energy Security mission area and Materials for the Future science pillar by studying and improving the radiation tolerance of ferritic alloys, which resist void swelling better than conventional alloys.

Arul Kumar received a 2015 Young Professional Poster award for “Modeling of shear transformation induced deformation behavior in crystalline materials” in the Structural Materials Division. Mentored by Carlos Tomé and Ricardo Lebensohn (MST-8), he used crystal plasticity-based materials modeling to explore the role of microstructure in the deformation behavior of hexagonal materials. He holds a PhD in mechanical engineering from the Indian Institute of Technology in India.



The DOE Office of Basic Energy Sciences E401 program funded the research, which supports the Laboratory's Global Security and Energy Security mission areas. The work also supports the Materials for the Future science pillar by devel-

oping an understanding of hexagonal close-packed materials, which are used in structural applications impacting nuclear reactor technology, automotive technology, aviation, and defense.

#### References:

- “Microstructure and mechanical property evolution during tube processing of oxide dispersion strengthened (ODS) ferritic steels,” Aydogan (Texas A&M University, MST-8), Osman Anderoglu, Stuart Maloy, Sven Vogel (MST-8), with collaborators from Texas A&M, University of California-Santa Barbara, Oak Ridge National Laboratory, Case Western Reserve University, and Ames Laboratory
- “Swelling resistance of several variants of ferritic alloy EK-181 at high doses during self ion irradiation,” Aydogan, with collaborators from Texas A&M, Moscow Engineering and Physics Institute, Bochvar Institute of Inorganic Chemistry, Institute of Physics of Advanced Materials and Nanocenter, University of Florida, Massachusetts Institute of Technology, and Radiation Effects Consulting
- “Modeling of Shear Transformation Induced Deformation Behavior in Crystalline Materials,” Arul Kumar, Carlos Tomé

*Technical contacts: Eda Aydogan and M. Arul Kumar*

### *Ellen Cerreta joins ASM Board of Trustees*

Ellen Cerreta will begin a three-year term as an ASM International Trustee this fall. The ASM Board of Trustees guides the course of the society—defining its ideals and activities, approving budgets, choosing the managing director, and advising ASM's top leadership. The board includes four officers and nine trustees.



Cerreta, who earned a PhD in materials science and engineering from Carnegie Mellon University, is the Materials Science in Radiation and Dynamics Extremes (MST-8) group leader. She studies dynamic damage due to shock loading and shear deformation of metals, leading research into the deterministic features of dynamic failure with the goal of developing damage-tolerant materials for aerospace, defense, automotive, and manufacturing applications. She has held leadership roles at Los Alamos, ASM, and TMS (The Minerals, Metals & Materials Society). She is vice-chair of the TMS Structural Materials Division and served on the TSM Board of Directors from 2009 to 2012.

ASM International is the world's largest association of metals-centric materials engineers and scientists. Metallurgy (MST-6) Characterization and Special Projects Team Leader and current ASM Trustee Jim Foley will end his three-year term this October.

*Technical contact: Ellen Cerreta*

## George “Rusty” Gray’s accomplishments recognized at TMS honorary symposium

Rusty Gray (Materials Science in Radiation and Dynamics Extremes, MST-8) was honored with a six-session symposium during TMS 2015, The Minerals, Metals & Materials Society’s (TMS) 144th annual meeting and exhibition, held in Florida. The meeting draws more than 4,000 business leaders, engineers, scientists, and other professionals in the materials field.



The Constitutive Response and Modeling of Structural Materials symposium was a forum for discussing recent investigations concerning structure/property relations within structural materials—the heart of Gray’s work. Primary focus areas included constitutive response/modeling of structural materials, characterization of microstructural, textural, and damage evolution; prediction and simulation of strength and damage evolution; and model validation and experimental support.

Ellen Cerreta (MST-8), Eric Brown (Neutron Science and Technology, P-23), Neil Bourne (University of Manchester, United Kingdom), James Williams (The Ohio State University), and Kenneth Vecchio (University of California, San Diego) organized the symposium, with sponsorship from the TMS Structural Materials Division and the Mechanical Behavior of Materials Committee.

Gray, who has a PhD in metallurgical engineering from Carnegie Mellon University, pursues fundamental and applied research primarily in the elucidation of the structure and property behavior of materials subjected to dynamic and shock-wave deformation. He was the 2010 TMS president, has served on TMS programming, titanium, and mechanical behavior committees, and on its board of directors as Structural Materials Division chair and director of publications. He has received the Structural Materials Division’s Distinguished Scientist/Engineer Award and is a Fellow of TMS, Los Alamos National Laboratory, the American Physical Society, and ASM International. Gray was recently re-appointed to a second, two-year term as chair of The National Academy of Sciences Panel on Ballistics Science and Engineering at the U.S. Army Research Laboratory (ARL). The panel annually reviews the scientific and technical quality of ARL ballistics science and engineering research and development programs, providing input to the ARL Technical Assessment Board for its biennial assessment report on the overall quality of ARL scientific and engineering research.

*Technical contact: Rusty Gray*

## Blas Uberuaga recognized for distinguished mentoring

Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8) has received a Los Alamos National Laboratory Postdoc Distinguished Mentor Award. The awards recognizes the positive impact and contributions a mentor makes during a postdoc’s appointment and are awarded to those who demonstrate a level of mentoring substantially beyond expectations.



MST-8 postdocs Pratik Dholabhai, Ghanshyam Pilania, and Satyesh Yadav nominated him.

Uberuaga mentors six postdocs and has previously successfully mentored more than a dozen postdocs at Los Alamos; five of which have become technical staff in industry, two have been converted to scientific staff at Los Alamos, two have joined other laboratories, and three have taken academic positions.

A dedicated mentor who improves his postdocs’ career portfolio and motivates them to become successful researchers, he accommodates, inspires, and trains culturally diverse postdocs with a variety of abilities and interests, and mentors them to pursue successful careers. As an experienced leader for several projects, he shares the importance of effective communications in scientific paper writing, technical presentations, and proposal writing. Uberuaga meets regularly with his postdocs, encourages them to think independently and establish new collaborations to gain visibility in the field, and provides postdocs with great freedom and encourages them to try new ideas that could lead to novel discoveries. When projects are successful, he displays remarkable humility and gives the credit to postdocs. This helps postdocs develop leadership abilities and gain visibility in scientific circles.

*Technical contact: Blas Uberuaga*



## TMS officials tour and discuss Laboratory's materials science expertise

Top leadership of The Minerals, Metals and Materials Society (TMS) learned about Los Alamos National Laboratory's wide-ranging materials research during a recent two-day visit to key Laboratory facilities and through discussions with Laboratory materials scientists.

Los Alamos National Laboratory has the largest number of TMS members of any organization represented in the materials professional society. The visitors were interested in learning more about the materials programs and capabilities at Los Alamos and gleaning feedback on how Laboratory employees could be better served by TMS.

TMS President Patrice Turchi, TMS Executive Director Jim Robinson, and *JOM* Contributing Editor Lynne Robinson began their visit with an overview of the Lab's strengths in materials science from Associate Director for Experimental Physical Sciences Mary Hockaday, followed by a tour of the Proton Radiography Facility at the Los Alamos Neutron Science Center. Invented at Los Alamos, proton radiography uses a high-energy proton beam from the LANSCE accelerator to image the properties and behavior of materials under a variety of conditions.

At the Lab's Materials Science Complex, the TMS visitors were shown a sampling of the capabilities available in the Sigma Complex. This 200,000-square-foot facility is unique in the Laboratory, and perhaps within the United States, providing a highly integrated approach where materials can be processed on a large scale from the raw state to a final product. This visit included stops at the foundry, machine shop, characterization and fabrication labs, additive manufacturing facilities, and Sigma's Electron Microscopy Laboratory.

At the Materials Science Laboratory, they met with Lab scientists, learning about Los Alamos's dynamic testing and single crystal growth capabilities, and research being performed at the Ion Beam Materials Laboratory and the Center for Integrated Nanotechnologies.



**David Alexander (center) of MST-6 discusses machining in the Sigma Complex with TMS President Patrice Turchi (left) and Amy Clarke (MST-6).**



**TMS Executive Director Jim Robinson (left) and TMS President Patrice Turchi examine an additive manufacturing part.**



**Cameron Knapp (left) of MST-6 reviews some of the Laboratory's additive manufacturing techniques and capabilities with TMS Executive Director Jim Robinson and *JOM* Contributing Editor Lynne Robinson.**

The visit also included a tour of the National High Magnetic Field Laboratory and the Power Wall in the Strategic Computing Complex.

In all, TMS leaders met with more than 20 scientists during their stay, which included a visit to the Bradbury Science Museum on the next day.

## Understanding the behavior of nanocrystalline materials in extreme environments

Los Alamos researchers used long-time simulation methods to determine the mobility of defects and defect clusters at a variety of grain boundaries in copper. The work reveals key factors that could allow scientists to improve the functionality of nanocrystalline materials in extreme environments, such as nuclear reactors, where the interfaces are expected to promote radiation tolerance. The journal *Scientific Reports* published the work.

The researchers used a combination of accelerated molecular dynamics, adaptive kinetic Monte Carlo, and object kinetic Monte Carlo to determine the mobility of defects at grain boundaries (GBs) and the impact on GB sink efficiency. They examined how the grain boundary structure changes both the mobility of isolated point defects and the behavior of defect clusters, focusing on the mobility of interstitial clusters as a function of cluster size at four representative GBs. Object kinetic Monte Carlo simulations probed the influence of the atomistic results on the sink efficiency of GBs.

The way different types of grain boundaries accommodate defects and thus how those defects move depends on the grain boundary character. The image shows the structure of a cluster of five interstitials at four different grain boundaries. The structures of these clusters differ significantly with grain boundary structure, and so too do the mobilities of those clusters. These differences have ramifications for the evolution of defects at and near the grain boundary under irradiation and thus the response of the entire material.

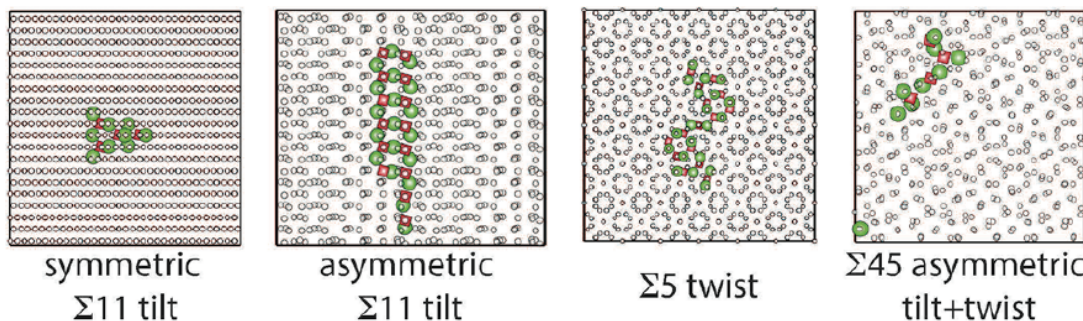
The researchers report that mobilities vary significantly with boundary structure and cluster size—the larger the cluster size, the less mobility—and that interface sink efficiency depends on the kinetics of defects within the interface. Thus, sink efficiency is a strong function of defect mobility, which depends on boundary structure, a property that evolves with time. Moreover, defect mobility at boundaries can be slower than in the bulk. This phenomenon has implications for the properties of polycrystalline materials more generally.

Depending on the rate at which damage is produced under irradiation (either by how fast incoming particles hit the material or the mass of the incoming particles), the nature of the produced damage will vary, from isolated point defects to clusters of defects. The simulations show that the mobility of point defects versus clusters of defects varies from

boundary type to boundary type. The object kinetic Monte Carlo simulations reveal that the response of the material as a whole is sensitive to these mobilities. Thus, the ability of different types of grain boundaries to mitigate radiation damage will depend on the irradiation conditions. Boundaries that lead to enhanced recovery when defect clusters dominate may not do so well when point defects are produced. This result suggests that the overall response of the material is not only a function of the types of grain boundaries present, but also the irradiation conditions.

Scientists know that interfaces, including GBs, can promote radiation tolerance by providing new avenues for defect annihilation. Prior experiments have revealed that different types of interfaces interact with defects more or less strongly. However, the origin of this dependence has remained elusive. These new simulations suggest that the rate of defect annihilation within the interfaces is an important factor. It has long been known that the rate of defect annihilation

in the bulk of the material dictates the overall defect content in large-grained materials. The new insight from these simulations indicates that the overall defect content



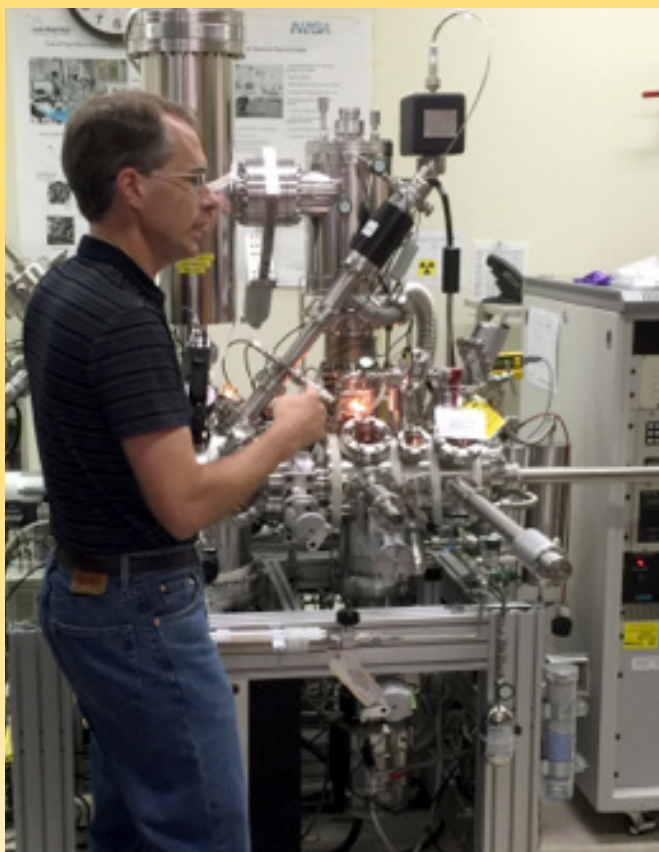
**Structure of a cluster of five interstitials at four different grain boundaries.**

in a nanocrystalline material is a competition of defect annihilation in the grain interiors and at the interfaces, which in turn is controlled by defect mobility within the interface, a property that depends on the interfacial character. Thus, the defect annihilation rate at the interfaces is a key property controlling the radiation tolerance in these materials.

Reference: “The Relationship between Grain Boundary Structure, Defect Mobility, and Grain Boundary Sink Efficiency,” *Scientific Reports* **5**, 9095 (2015). Authors include: Blas Uberuaga and Enrique Martinez Saez (Materials Science in Radiation and Dynamics Extremes, MST-8), Louis Vernon (Applied Computer Science, CCS-7), and Arthur Voter (Physics and Chemistry of Materials, T-1). The Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the DOE, Office of Science, Office of Basic Energy Sciences (BES) sponsored the work in part. The DOE BES, Materials Science and Engineering Division funded Voter. The research supports Los Alamos National Laboratory’s Energy Security mission area and Materials for the Future science pillar through study of the effect of extreme environments on materials.

*Technical contact: Blas Uberuaga*





Tom Venhaus (Nuclear Materials Science, MST-16) describes the time-of-flight secondary ion mass spectrometer used for actinide corrosion studies at the Target Fabrication Facility.

## Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries recently:

Manuel Lovato, MST-8 .....	40 years
Ross Muenchausen, MST-7 .....	30 years
Angela Martinez, MST-8 .....	10 years
Jacob Sutton, MST-6 .....	10 years
Raja Chellappa, MST-8 .....	5 years
Samrat Choudhury, MST-8 .....	5 years
Graham King, MST-8 .....	5 years
Enrique Martinez Saez, MST-8 .....	5 years

## HeadsUP!

### Work planning and biological safety assessment

Members of the Department of Energy's Office of Environment, Safety and Health Assessments Office of Enterprise Assessments recently toured several programmatic areas within MST.

Their visit was one of the Office's periodic reviews of the Laboratory's work planning and control and biological safety program.

The four-day visit included stops in the Sigma Facility, Target Fabrication Facility, the Material Science Laboratory, the Health Research Laboratory, and the Bio-Safety Level-3 facility as well as overview briefings on the mission and history of the facilities and the research performed. They plan to return in mid-July for another four-day visit.

## MSTeNEWS

Materials Science and Technology

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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or [kkippen@lanl.gov](mailto:kkippen@lanl.gov).

To read past issues, see [www.lanl.gov/orgs/mst/mst\\_eneews.shtml](http://www.lanl.gov/orgs/mst/mst_eneews.shtml).



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